

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

| Weighted KNN model | | | | | |
|--------------------|------|----------------|------|------------|------|
| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 1.14 | 0.85 | 1.12 | 0.83 | 1.23 |

Model Results

Predicted value: 3.76e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.44e-01

Confidence level: 6.65e-01

Nearest Neighbors from the Training Set

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2-Methyl-p-benzoquinone

Measured: 2.35e-11

Predicted: 2.15e-11

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alpha-Humulene

Measured: 2.90e-10

Predicted: 2.87e-10

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1,4-Naphthoquinone

Measured: 3.10e-12

Predicted: 3.16e-11

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(3Z)-3-Hexenyl acetate

Measured: 7.80e-11

Predicted: 7.52e-11

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80e-11

Predicted: 4.73e-11